MULTIBAND MODEL OF HIGH Tc SUPERCONDUCTORS

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We propose an extension to other high T_c compounds of a model introduced earlier for YBCO. In the "self-doped" compounds we assume that the doping part (namely the BiO, HgO, TlO planes in BSCCO, HBCCO, TBCCO respectively) is metallic, which leads to a multiband model. This assumption is supported by band structure calculations. Taking a repulsive pairing interaction between these doping bands and the CuO_2 bands leads to opposite signs for the order parameter on these bands and to nodes whenever the Fermi surfaces of these bands cross. We show that in BSCCO the low temperature dependence of the penetration depth is reasonably accounted for. In this case the nodes are not located near the 45^o direction, which makes the experimental determination of the node locations an important test for our model. The situation in HBCCO and TBCCO is rather analogous to BSCCO. We consider the indications given by NMR and find that they rather favor a metallic character for the doping bands. Finally we discuss the cases of NCCO and LSCO which are not "self-doped" and where our model does not give nodes.

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I. INTRODUCTION

The recent years have seen a marked progress in the debate on the mechanism of high T_c superconductivity. Indeed the existence of nodes and change of sign of the order parameter at the Fermi surface has found a very important experimental support in some compounds like $YBa_2Cu_3O_7$ (YBCO) . This includes on one hand various experiments showing the existence of low energy excited states, such as tunneling, Raman scattering and penetration depth [1]. Moreover more spectacular experiments designed to probe the change of sign have given positive answers. These are the corner SQUID experiments [2] and the observation of the half magnetic flux quantum in 3 grain-boundary Josephson junctions [3]. This change of sign is a clear indication that there is some important repulsive contribution in the pairing interaction. Since the spin fluctuation mechanism [4] is based uniquely on a repulsive interaction, it appears as a leading candidate for the pairing mechanism in these high T_c superconductors. In its simplest version it leads to an order parameter with a $d_{x^2-y^2}$ symmetry, commonly called d-wave order parameter.

Unfortunately this simple spin fluctuation interpretation meets some problems in YBCO. An important one is the weak sensitivity of the critical temperature of $YBa_2Cu_3O_7$ to defects. Any kind of impurities produces in d-wave superconductors an effect analogous to pair-breaking by magnetic impurities in standard s-wave superconductors, leading to a rapid decrease of the critical temperature with increasing scattering rate, as measured for example by the residual resistivity. This is in contrast with some experiments showing a decrease of T_c an order of magnitude slower than expected [5].

Another problem is the marked anisotropy in the a-b plane shown by a number of recent experiments in YBCO. The existence of a sizeable Josephson current [6] in a c-axis $Pb - YBa_2Cu_3O_7$ tunnelling junction shows that pure d-wave symmetry is not satisfied. Because of the large size of this Josephson current as compared to what would be expected from a superconductor with s-wave symmetry, it is difficult to believe that the departure from pure d-wave is only due to the small orthorhombic 1,6% distorsion of the CuO_2 planes. Various other properties have also shown a clear in-plane anisotropy. The resistivity has an anisotropy of about a factor 2. Quite recently a sizeable anisotropy of the thermal conductivity has been observed [7] which reaches 30% in the superconducting state.

The anisotropy of the penetration depth is perhaps the most striking one since it is directly related to the nature of the superconducting state. Indeed [8] at zero temperature, the ratio between the superfluid densities $\lambda_b^{-2}(0)/\lambda_a^{-2}(0)$ is 2.3 , which is in good agreement with the anisotropy of the normal state resistivity and of the square of the plasma frequency [8]. Moreover we have also to take into account that in $YBa_2Cu_4O_8$, which has twice as many chains as $YBa_2Cu_3O_7$ and an orthorhombic distorsion of 0.8% , the superfluid density anisotropy [8] is as high as 6.2 . This trend points toward the natural conclusion that the chains are conducting and that the superfluid density anisotropy is due to their direct contribution. Now we attribute the linear term at low temperature to nodes in the gap. Since in $\lambda_b^{-2}(T)$ this linear term is typically 3 times the linear term in $\lambda_a^{-2}(T)$, the nodes contribution is also strongly anisotropic.

This leads to the suspicion that chains have also something to do with the nodes. This is not so easy to include in the spin fluctuation picture because it deals only with the CuO_2 planes. This gives rather a strong hint that we have to include chains explicitely in our modeling of the superconducting state in order to come up naturally with such an anisotropy. Another strong indication that chains play an important role in the superconducting properties comes from very recent penetration depth measurements [9] which are partially in contradiction with earlier results [10], and show a kink in the temperature dependence. This seems to indicate that a two component model is appropriate for the description of superconductivity and leads again to a two band model. Naturally the present overall experimental picture is still somewhat uncertain and future experiments will help to clarify the situation.

These difficulties, as well as others, with the spin fluctuation mechanism have led us to propose recently a model [11] which allows to account for all the above experimental facts. In this model pairing in the planes is due to an attractive interaction, while Coulomb repulsion induces in the chains an order parameter with opposite sign. It is well known that these plane and chain bands hybridize because electrons are physically allowed to jump from planes to chains. Due to the anticrossing produced by this hybridization, one obtains automatically an order parameter which changes sign on a single sheet of the Fermi surface and has nodes in the gap in the region of the Brillouin zone where the anticrossing takes place. In this sense our order parameter is d-wave like. However in contrast with the $d_{x^2-y^2}$ order parameter, there is no symmetry breaking and we have a total of 8 nodes (4 on each sheet of the Fermi surface) instead of 4. Since the chains play an essential role in our model, it is meaningless to consider an approximate tetragonal symmetry. Rather we have to consider only the orthorhombic symmetry, under which our order parameter is completely invariant (no symmetry breaking), which is also the case for the $d_{x^2-y^2}$ order parameter . We can also say that on each sheet of the Fermi surface our order parameter looks qualitatively like a d+s order parameter.

Since the order parameter of our model has nodes, it accounts naturally for all the experiments providing evidence for its change of sign and for the existence of low energy excitations. At the same time it provides also a simple explanation for the important anisotropy in the ab plane mentionned above, because of the important role of the chains. We have found [12] that the existence of two weakly coupled bands (plane and chain) in our model, as well as weak plane-chain scattering, leads to the possibility of a weak sensitivity of the critical temperature to impurities, in agreement with experiment. We find [13]that our model accounts quite well for the anisotropy of the penetration depth and for the absolute values. We are also able to reproduce fairly well the whole temperature dependence for both the a and the b directions found in Ref. [10], including the linear dependence at low temperature.

Although our model is quite satisfactory for YBCO, in part because there are strong experimental indications that chains play a significant role, it appears for the same reason quite specific of YBCO and does not seem to be applicable to other compounds. However the natural tendency is to find a universal explanation for high T_c superconductivity and hence a model applicable to all cuprate superconductors, since they all share fairly high T_c and CuO_2 planes. On this basis our model sounds quite unsatisfactory. Let us merely remark that fortunately this universality hypothesis can be checked and hopefully will be checked experimentally. We note also that the available data do not seem to confirm completely this hypothesis, since $Nd_{2-x}Ce_xCuO_4$ (NCCO) on one hand and YBCO (for the strong anisotropy discussed above) on the other do not fit in the picture. The case of NCCO will be discussed below. It would clearly not be satisfactory to find models specific to each of the different high T_c compounds, but it is possible that, while sharing common features, they also differ in some respect. A related unappealing feature of our model is its complexity, since it is basically a two band model, not as nice as a one band model. Ideally one would certainly rather like to have a simple rather than a complicated model. However we already know that these compounds are chemically complicated. The same might unfortunately be true for their physics.

Whatever the feeling about the above issues, there remains a more practical question. Other high T_c compounds have been investigated experimentally and have shown features similar to the ones found in YBCO (although the experimental picture is not as complete as in YBCO). Is it possible to extend the ideas of our model and find satisfactory explanations for them ? And more generally, following these ideas, what do we expect to find in other compounds ? It is the purpose of this paper to consider this question. As we mentionned our model for YBCO is basically a multiband model. Therefore we will in particular consider whether a multiband model is applicable to a given compound and if this can lead to reasonable explanations for experimental facts. We note that a multiband model applies trivially in all the compounds having more than one CuO_2 plane in the elementary cell. The usual trend is to consider that this leads to almost degenerate bands and to treat them as a single band. It is not completely obvious that this is correct, but anyway this will not be our main emphasis. We will rather be interested in looking if there are bands, analogous to the chain band of YBCO, that is not linked to the CuO_2 planes, which play physically an important role. Naturally we do not intend to review the whole situation but only to make our best to discuss what we believe to be relevant points. Our conclusion is that we can extend our model in a natural way and we do

not find major incompatibility with experiments. Naturally this is a somewhat imprecise statement and we will be more specific below. We consider successively the cases of BSCCO, HBCCO, TBCCO, and finally LSCO and NCCO.

II. BSCCO

We turn first to the extension of our model to $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), which is probaby the second most investigated high T_c superconductor after YBCO. This is not a very good compound for fundamental investigations since it is generally not stoechiometric but rather has often an oxygen "doping" δ giving the maximum T_c . This comes in addition to the incommensurate distorsion arising in the BiO planes. This is in contrast with YBCO where the nearly stoechiometric compound has been mostly investigated. We first note the high value of $2\Delta/T_c$ (which is of order 7 or even higher, as obtained from tunnelling experiment [14] as well as from Raman scattering [15]) gives an indication that a simple d-wave model does not properly describe BSCCO. This value is incompatible with a weak coupling d-wave model, and it is doubtful that strong coupling spin fluctuations calculations [16] can lead to such a high value, because the spectrum for spin fluctuations goes to high energy and the coupling constant is of order unity. A related difficulty is the value of the slope of the penetration depth $\lambda(T)$ at low temperature [17,18]. In the μ model of Xu et al. [19], which is an extension of the simple d-wave model allowing for a variable slope for the opening of the gap, $\Delta(\theta) = \Delta_0\ \mu\ \theta$ for $0 < \theta < \mu^{-1}$ and $\Delta(\theta) = \Delta_0$ for $\mu^{-1} < \theta < \pi/4$. The low temperature $\lambda(T)$ is given by [19]: [$\lambda(T)$ - $\lambda(0)$] / $\lambda(0)$ = (2 ln2 / $\mu\ \Delta_0$) T . Taking the experimental value $\lambda(T)$ - $\lambda(0) \approx 10$ Å / K and $T_c \approx 90$ K , this leads to $\mu\ \Delta_0\ /\ T_c = 1.5\ 10^{-3}\ \lambda(0)$, where $\lambda(0)$ is measured in Å . There is some uncertainty in $\lambda(0)$. If we take the assumed values of 2100 Å [18] and 2600 Å [17], we have either $\mu\ \Delta_0\ /\ T_c \approx 3.2$ or $\mu\ \Delta_0\ /\ T_c \approx 4$. Taking the (pretty unphysical) lower limit $\mu = 4\ /\pi$ leads to $2\Delta_0\ /\ T_c = 5$ or 6.2 , somewhat below experiment. The standard d-wave corresponds essentially to $\mu = 2$ and gives $2\Delta_0\ /\ T_c = 3.2$ or 4 , barely compatible with weak coupling and in clear disagreement with experiment. It might naturally be that further experiment give a higher value for $\lambda(0)$ and a lower one for $2\Delta/T_c$ which would solve this difficulty.

The natural way to extend our two-band model to BSCCO is to assume that the BiO planes lead to a metallic band, which would play the role of the chain-band in YBCO. The existence of this band at the Fermi level is controversial. There is some experimental evidence from photoemission that BiO planes are insulating because the BiO band is not seen [20], but these experiments are somewhat contradictory [21]. Similarly STM seems to indicate that the BiO plane at the surface is nonmetallic [14]. However both kind of experiments test only the surface of the sample on a few tens of Å, that is basically one cell depth. Just because the surface necessarily implies some kind of lattice distorsion and/or consequently some modification in the electronic spectrum, the BiO planes may well be insulating at the surface while they are conducting in the bulk. It may also very well be that there is some oxygen depletion at the surface. An example of this kind of problem is found in YBCO [22]. In this compound the bands corresponding to CuO_2 planes are seen in photoemission, while the CuO chain-derived band is not seen. This could lead again to the conclusion that this chain band is nonmetallic. However this chain band is seen by ACAR (which does not see the plane bands) which shows that this band is metallic. As indicated above this is confirmed completely independently by the in-plane anisotropy of the conductivity and mostly by the strong anisotropy of the superfluid density. Other problems arising with the interpretation of photoemission experiments are discussed in [1].

The main reason to believe that the BiO planes are metallic comes from band structure calculations [23,24]. Indeed these papers find that, in addition to the two nearly degenerate CuO_2 plane-derived bands, there is at the Fermi level a BiO-derived band. The plane bands are rather similar to the ones found in YBCO, and the corresponding Fermi surface looks roughly as a circle centered at ($\pm\ \pi$ / a , $\pm\ \pi$ / a) if one uses the simplified Brillouin zone corresponding to tetragonal CuO_2 planes. The BiO band gives a smaller Fermi surface centered at ($\pm\ \pi$ / a , 0) and (0 , $\pm\ \pi$ / a). Naturally one may wonder about the validity of band structure calculations. Clearly there are limitations in the precision of these complicated calculations. They are also sensitive to the precise location of the atoms. And LDA, which is commonly used to take into account correlations, is not an exact method for dealing with highly correlated systems. As a result mass renormalization due to interactions is not included and the calculations provide essentially the bare excitation spectrum (note however that mass renormalization due to Coulomb interaction seems to be rather small, from all the calculations dealing with correlation effects). On the other hand the results from different authors are in fair agreement, which indicates at least that the results are reasonably well converged. Moreover in the case of YBCO, the results are in reasonable agreement with all experimental informations from ARPES, ACAR and dHvA [22], including a small electron pocket centered at ($\pm\ \pi$ / a , $\pm\ \pi$ / a) , which is apparently not of physical importance. It is therefore difficult to ignore these results and one has to consider seriously the possibility that their conclusion is correct.

In the case of BSCCO the BiO band is mostly above the Fermi level, but the bottom of the band is located around 0.5eV below the Fermi level. It is likely that the precision of the method is better than this, and the BiO band will not be pushed above the Fermi level by some imprecision in the calculations. Therefore the existence of this BiO Fermi surface seems rather secure. On the other hand the calculations show a second BiO band which comes quite close to the Fermi level from above (within 0.1eV or less), but does not cross it. It is not obvious that the precision is good enough to make sure that there is not a second BiO sheet of the Fermi surface. Experimentally, as mentionned above, ARPES does not see the BiO band, but it sees the CuO_2 bands (or at least one of them, but the failure to see two bands might be due to their splitting being very small). The Fermi surface corresponding to this band is in good agreement with band structure calculations, which gives again confidence in these calculations. On the other hand ACAR [25] gives results in fair agreement with band structure calculations and sees the BiO piece of the Fermi surface, although its size is somewhat larger than the theoretical prediction and the separation between BiO and CuO_2 Fermi surfaces larger than predicted. Recent experiments [26] on the mid-infrared reflectivity in $Bi_2Sr_2CuO_6$ have also been interpreted in terms of transitions between BiO and CuO_2 type bands. As mentionned above the discrepancy with ARPES might be due to the fact that the surface structure is different from the bulk. A similar problem may be seen in Sr_2RuO_4, a layered perovskite becoming superconducting around 1K. Here there is some disagreement between ARPES [27] and dHvA [28] experiments, and it has been suggested [29]that the origin might be surface relaxation of the oxygen position.

Actually calling this electron pocket the BiO piece of the Fermi surface is a misnomer. Indeed the corresponding electronic states are [23,24] strong hybrid of states describing electrons moving respectively in BiO planes and in CuO_2 planes. The situation is quite similar to the one found in YBCO where we start with electrons belonging either to planes or chains, and which are hybridized due to the hopping of an electron from plane to chain, through the apical oxygen. In the same way we can start in BSCCO with "non-interacting" bands, as considered explicitely by Massida et al. [24], corresponding to electrons moving either in BiO planes or in CuO_2 planes. Then hopping through the apical oxygen produces an hybridization of these bands [24]. The net result is that [24] the BiO planes contribution to the total density of states at the Fermi level is almost half of the one of the CuO_2 planes, which shows clearly the importance of BiO planes.

It is possible to produce semiquantitatively the results of band structure calculations with a simple tight-binding model. Let us indeed consider that BSCCO is build by stacking up sets made of two CuO_2 planes and two BiO planes. Motion in the CuO_2 planes and in the BiO planes is described by the dispersion relations ϵ_k and ϵ'_k respectively. Moreover we allow hopping toward the nearest plane. We call t the hopping term between a CuO_2 plane and the nearest BiO plane, t' the hopping term between the two BiO planes and t" the one between the two CuO_2 planes, assuming for simplicity that they are wavevector independent. The corresponding Hamiltonian is:

$$\begin{aligned} H_0 = &\sum_n \varepsilon_k c^+_{k,1,n} c_{k,1,n} + \sum_n \varepsilon_k c^+_{k,2,n} c_{k,2,n} + \sum_n t" \, (c^+_{k,1,n} c_{k,2,n} + h.c.) \\ &+ \sum_n \varepsilon'_k d^+_{k,1,n} d_{k,1,n} + \sum_n \varepsilon'_k d^+_{k,2,n} d_{k,2,n} + \sum_n t' (d^+_{k,1,n+1} d_{k,2,n} + h.c.) \\ &+ \sum_n t (c^+_{k,2,n} d_{k,1,n} + h.c.) + \sum_n t (c^+_{k,1,n} d_{k,2,n} + h.c.) \end{aligned} \tag{1}$$

where c^+_k and d^+_k are creation operators in the CuO_2 planes bands and in the BiO planes bands respectively. The indices 1 and 2 number the CuO_2 planes and BiO planes, while the index n numbers the stacks. Actually we can simplify further by taking into account that BSCCO is very anisotropic which implies that some hopping terms are quite small. From band structure calculations [23] it is clear that hopping between CuO_2 planes and between BiO planes are small, while hopping between neighboring CuO_2 plane and BiO plane are somewhat stronger, leading to rather isolated CuO_2 - BiO stacks. For simplicity we assume for example hopping between BiO planes negligible, that is t' = 0, and t" $\neq$ 0 . But we could take the opposite assumption t' $\neq$ 0, and t" = 0 and reach the same qualitative conclusions. The important point is that the sets made of two CuO_2 planes and two BiO planes are now independent and we have a two-dimensional problem. The Hamiltonian can then be separated in two independent parts $H_\pm$ corresponding to even and odd combinations. Introducing the operators $c_\pm$ and $d_\pm$ by $c_{1,2} = (c_+ \pm c_-)/\sqrt{2}$ and $d_{1,2} = (d_+ \pm d_-)/\sqrt{2}$:

$$H_\pm = \sum_k (\varepsilon_k \pm t") c^+_{k,\pm} c_{k,\pm} + \sum_k \varepsilon'_k d^+_{k,\pm} d_{k,\pm} + \sum_k t (c^+_{k,\pm} d_{k,\pm} + h.c.) \tag{2}$$

Each of these Hamiltonian is analogous to the two-dimensional model [11] we have considered for YBCO. For each of them the CuO_2 band and the BiO band hybridize. Since band structure calculations show that one of the BiO derived

band is pushed above the Fermi level by this coupling, we consider only the other Hamiltonian, where hybridization leads to an anticrossing of the Fermi lines. In order to obtain a Fermi surface in reasonable agreement with band structure calculations, we take for the unhybridized CuO_2 band the rather standard dispersion relation : ϵ_k - t" = - $2t_0$ (cos($k_x a$) + cos($k_y a$)) + $2t_0$ cos($k_x a$) cos($k_y a$) - μ with t_0 = 0.33 eV, μ = - 0.46 eV (the axes are along the CuO bonds). On the other hand the unhybridized BiO band can be described by a nearest neighbour tight binding approximation (with BiO bonds rotated by 45^o with respect to the CuO bonds), which leads to $\epsilon'_k = 4t'_0$ cos($k_x a$) cos($k_y a$) - μ' , with t'_0 = 0.3 eV and μ' = - 0.6 eV in order to reproduce band structure calculations. The result for the Fermi lines is shown in Fig.1 for t = 0.1 eV . This figure is very similar to the Fermi surfaces found in [23,24]. We can then take over our model [12] for YBCO and assume that there is a repulsive pairing interaction between CuO_2 plane and BiO plane, leading to an order parameter with opposite sign in the CuO_2 plane and BiO plane. Then because of hybridization we have nodes in the anticrossing regions. To give an example we assume the regime of well separated bands, where the hopping term t is large compared to the gaps (actually it is not clear that this condition is satisfied because the maximum gap is quite large in BSCCO as we have seen above, but this should not lead to qualitative changes). In this case, assuming for simplicity isotropic order parameters Δ in the CuO_2 plane and Δ' in the BiO plane, the order parameter is given [12] by Δ_k = (Δ ϵ'_k + Δ' ϵ_k) /(ϵ_k + ϵ'_k) when hybridization is taken into account. In particular the locations of the nodes is not so sensitive to the ratio Δ/Δ' because the Fermi lines for unhybridized CuO_2 plane and BiO plane cross essentially at right angle. We show in Fig.1 the locations of the nodes for Δ/Δ' = - 1 .

We can then try to calculate the temperature dependence of the penetration depth, just as we have done for YBCO [13]. However the results depend sensitively on a number of ingredients [13] and the situation is here much more uncertain than in YBCO, in particular with respect to the band structure and the parameters describing the BiO derived bands. Therefore we will only consider the low temperature behaviour where the number of hypotheses can be somewhat more limited. We proceed as in [13] and treat the hopping term t as a small quantity so that hybridization modifies the dispersion relations only in the vicinity of the crossing of the unhybridized Fermi lines. This leads to :

$$\lambda^{-2}(0) - \lambda^{-2}(T) = \frac{4 \ln 2}{\pi} \frac{e^2 \mu_0}{\hbar^2} \frac{t}{c} \frac{T}{(\Delta \, |\Delta'|)^{1/2}} A_0 \tag{3}$$

where Δ and Δ' are the order parameters in the unhybridized CuO_2 and BiO planes respectively (which we have assumed to be **k**-independent for simplicity) and c = 14.6 Å is the thickness of the stack made of two CuO_2 planes and two BiO planes. The dimensionless constant A_0 is related to the quasiparticle velocities at the crossing point of the unhybridized Fermi lines. We assume for simplicity that these velocities are orthogonal (this is essentially the case in Fig.1). In this case A_0 is given by $A_0 = (\Delta^2 \, v_B^2 + \Delta'^2 \, v_C^2 \,)/(\Delta \, |\Delta'| \, v_B \, v_C)$ where v_C and v_B are the velocity of the unhybridized CuO_2 and BiO bands respectively. This quantity has a minimum equal to 2 when $\Delta \, v_B = |\Delta'| \, v_C$ and we take for simplicity this worst case for our evaluation. Expressing numerically all known physical constants, this can be rewritten in the low T regime as :

$$\lambda(T) - \lambda(0) = 2.8 \lambda^3(0) \frac{T}{T_c} \frac{T_c}{(\Delta \, |\Delta'|)^{1/2}} t \tag{4}$$

where the all penetration lengths are now expressed in units of 1000 Å and the hopping parameter t is in eV. We want now to compare this result with experiments [17,18] on BSCCO which gives a slope of 10 Å/K. We take for example Δ/Δ' = - 1 (actually we would expect Δ' to be somewhat less than Δ, which would be make our case easier), and $\lambda(0)$ = 2000 Å from experiment (again a rather worst case hypothesis). If we use $\Delta/T_c \approx 3$ as discussed above, we obtain agreement with experiment for t = 0.12 eV . This result is quite similar to what we have found for YBCO. It is small enough to make our hybridization approach consistent. This is quite satisfactory since we have basically no adjustable parameters. On the other hand it is not in contradiction with the strong anisotropy and the large resistivity well known in BSCCO, since this can be attributed entirely to the very small hopping between either the BiO planes or the CuO_2 planes or both, as we have already discussed. It may seem rather strange that we can account for the rather strong slope found experimentally by a small hybridization. Roughly speaking this is due to the fact that we have a total of 16 nodes in the Brillouin zone, whereas the standard d-wave model has only 4 nodes.

Our model differs clearly from standard d-wave, not only by the number of nodes but also by their locations. This is in contrast with YBCO where the location of the crossing between plane and chain bands is not so far from the 45^o direction of the standard d-wave model. Here, in Fig.1 , the directions of the nodes are respectively 18^o and 22^o (and all the other ones obtained by tetragonal symmetry), with the origin taken at (π, π) as it is usually done. This is quite different from the 45^o of the d-wave model. Naturally Fig.1 is just an example, and it is likely that the situation in actual BSCCO is somewhat different because band structure (as suggested by ACAR experiments)

and order parameter are not the ones we have chosen. However we do not expect the location of the nodes to change qualitatively. Therefore experiments designed to ascertain the position of the nodes are quite important and we consider now briefly the evidence for this position in BSCCO (we will also discuss this point below for HBCO). At first photoemission experiments were interpreted [30] as showing nodes at 35^o. Taking together into account experimental and theoretical uncertainties, we would not consider this as being in clear contradiction with our model. However these experiments have then been reinterpreted [31] as giving the nodes at 45^o which agrees with d-wave and disagrees with our model. Anyway, as we discussed above, it is not clear at all that photoemission provides a faithfull picture of what is happening in the bulk. And it sees only a CuO_2 derived band, and no BiO band. So the fact that our model disagrees with photoemission is not so surprising.

On the other hand in-plane tunneling experiments give an indication on the location of the nodes. They have shown a clear gap anisotropy [32]with a minimum gap along the CuO bond direction in contrast with photoemission experiments. Naturally, just as photoemission, this technique is limited in angular resolution and can not by itself display nodes, but the obvious conclusion is that the nodes of the gap are not so far from the CuO bond direction, if there are nodes at all in BSCCO. This is not in agreement with d-wave and more in favor of our model. Finally half-integer flux quantum effect has been observed in tricrystals of BSCCO [33], providing rather convincing evidence for a change of sign of the order parameter on the Fermi surface. However this experiment does not provide a unique answer for the location of the nodes. For example, although the geometry is essentially the same as the one used for YBCO and is therefore consistent with d-wave, a g-wave order parameter $\Delta(\theta) \approx \cos(4\theta)$ is also a possible solution. More generally, since the Josephson junctions (and in particular the scattering at the interfaces) are not controlled in the tricrystals, it seems quite difficult to be secure about the position of the nodes from this kind of experiments. In conclusion it is fair to say that the problem of locating the nodes in BSCCO is not at all settled. At the same time it would clearly be a crucial piece of information to know in a reliable way this location since this would definitely allow to narrow the number of possible models and be another step toward identifying the mechanism of high T_c superconductivity.

III. HBCCO

Let us consider now the case of the Hg compounds. Band structure calculations give a more complex situation than for BSCCO. Indeed the compound $HgBa_2CuO_{4+\delta}$ (Hg-1201) is found to have only a CuO_2 derived band crossing the Fermi level [34–37], although there is a HgO derived band which is coming quite near (typically 0.1 eV) to cross also the Fermi level from above. It is not clear that the precision of the calculations is enough to be certain about it. Moreover the role of oxygen doping, which is held responsible for the metallic and superconducting properties of this compound [34], is also difficult to take into account and it seems to be quite important [38]. Therefore it will be quite interesting to see what experiment will tell in this respect. The present tunneling data [39] are more in favor of a standard BCS density of states. This is coherent with our model since, with a single band, we expect only anisotropic s-wave pairing. However a two-band model is still an open possibility in this compound. An indication in this direction seems to be that, for Hg nuclei, T_1 has essentially the same value at T_c for Hg-1201 and Hg-1212, showing a similarity between these two compounds.

Indeed calculations in $HgBa_2CaCu_2O_{6+\delta}$ (Hg-1212) and $HgBa_2Ca_2Cu_3O_{8+\delta}$ (Hg-1223) find [40,35,36] the HgO derived band crossing also the Fermi level, in addition to the CuO_2 bands, which makes these compounds "self-doped". The situation is actually quite similar to the one found in BSCCO. The Fermi surface displays a small electron pocket centered at the X point. Because of hybridization between HgO and CuO_2 bands, the electronic states on this sheet of the Fermi surface have a mixed HgO - CuO_2 character, as well as those of the nearby CuO_2 bands in the vicinity of the X point. An anticrossing is clearly seen. Therefore the necessary ingredients for our model are present, just as in BSCCO, and they can lead in the same way to nodes in the gap. Experimentally Raman scattering on Hg-1212 [41]gives evidence for nodes in the gap, but it shows also that some nodes (if not all) are away from the 45^o direction. This is in disagreement with d-wave and in agreement with our model. The low temperature dependence of the in-plane penetration depth in Hg-1223 [42]seems to be linear, which would indicate the existence of nodes in the gap. The available tunneling [43] data are also suggestive of nodes. To summarize the present situation in these Hg compounds is coherent with our model.

IV. TBCCO

We consider finally the case of the Tl compounds. Here again band structure calculations give results quite similar to the ones found for Hg compounds. There is a TlO band which crosses [44–47] the Fermi level for $Tl_2Ba_2Ca_{n-1}Cu_nO_{4+2n}$ with n=1,2,3 and 4, giving rise to a small electron pocket for the Fermi surface. However for $Tl_2Ba_2CuO_6$ there is some disagreement between various calculations [44,47] and this result seems to be within the error bars. There are differences with Hg compounds. First the electron pocket is found around the Γ point. The states corresponding to this part of the Fermi surface are fairly delocalized throughout the cell with contributions not only from Tl and O atoms, but also from the apical O and even the $d(z^2)$ orbital of Cu atoms (as a result, for $Tl_2Ba_2CuO_6$ [47], this piece of the Fermi surface has a more pronounced 3-dimensional character). Then there is also the possible existence of hole pockets [44,45], derived from flat CuO_2 bands. Finally since one has always the problem of dealing with oxygen doping, compounded with the experimental uncertainty on the atomic positions, the band structure situation is quite complicated.

We can again apply our model as in the case of BSCCO and say that Coulomb repulsion will lead to an order parameter with opposite signs on the sheets of the Fermi surface linked to the CuO_2 band and to the TlO band. This might explain the observation [48] of spontaneously generated half quantum flux in $Tl_2Ba_2CuO_{6+\delta}$ tricrystals. Nevertheless a major difference in the results of band structure calculations as compared with the Bi and Hg compounds is the lack of crossing of the CuO_2 and the TlO bands. Therefore in our model we would not expect nodes to appear. However it might very well be that the experimental situation is in this respect slightly different from the one predicted by band structure calculations [44,47] and that there is actually some crossing. This possibility has also been considered in the context of the inter-layer pairing mechanism [49]. As we have mentionned there is enough uncertainty in the band structure calculations to allow for this possibility. Clearly direct information from ARPES, ACAR,dHvA experiments would be quite useful in order to settle this question. In our model these crossings would lead to nodes in the gap, in a way analogous to what we have found in BSCCO and HBCO. Actually available Raman scattering experiments [50] favor the existence of nodes in a way very analogous to HBCO since they give, in B_{1g} symmetry, a response linear in frequency at low ω, in the superconducting phase.

V. NMR

Since our model requires two kind of metallic bands in the Bi, Hg and Tl compounds, it appears important to find experimentally if we are indeed in this situation or not. This is actually rather difficult. We have already discussed this problem for BSCCO and found that there is no good experimental evidence against metallic BiO planes. Naturally one would rather like to find experiments proving definitely that they are indeed metallic, but we are not aware of any. Surprisingly the (quasi) quadratic structure of these compounds is in this respect a disadvantage, since in the case of YBCO the most reliable evidences of the metallic character of the chains come from the anisotropic properties linked to the orthorhombic structure. The difficulty comes from the microscopic nature of the information we are looking for, since for any macroscopic property we will not be able to know which one of the two bands is responsible for it.

Nevertheless it would seem that the NMR is an effective experiment in order to obtain this information since it is a local probe. The case of YBCO is a good example of this [51], although it seems to be somewhat forgotten. Indeed the superconducting transition is clearly seen as a strong drop both in the Knight shift K and in the relaxation rate $1/T_1$ of Cu(1) nuclei of the CuO chains, and the behaviour below T_c is qualitatively similar to what is observed for Cu(2) in the CuO_2 planes. This shows that there is on this Cu(1) site a non vanishing amplitude for the wavefunction of the quasiparticles subject to the superconducting condensation. Moreover the quantitative temperature dependence for Cu(1) below T_c is clearly different from the one observed for the planes Cu(2), both for K and $1/T_1$. This shows that what is seen by Cu(1) nuclei is not merely a transferred part of the wavefunction of quasiparticles located dominantly in the CuO_2 planes, since in this case we would expect the temperature dependence to be the same for Cu(1) and Cu(2). Therefore the NMR favors a two-band picture for YBCO. This picture is also supported by the fact that the magnitude of $1/T_1$ at T_c are quite similar for Cu(1) and Cu(2), and the same is true for the change in Knight shift between T = 0 and T_c .

Let us consider the situation for Hg compounds. ^{199}Hg NMR experiments have been performed recently [52]on $HgBa_2CuO_{4+\delta}$. Below T_c they display a strong drop both in the Knight shift K and in the relaxation rate $1/T_1$, so the Hg nuclei see the superconducting electrons. Moreover for ^{199}Hg , T_1T is essentially constant in the normal

state (the Knight shift is also constant with a "Korringa ratio" rather near what is expected from a Fermi liquid), whereas $(T_1T)^{-1}$ increases markedly with decreasing temperature for ^{63}Cu. This is in favor of a two-band picture, just as in YBCO. One may argue that antiferromagnetic fluctuations are responsible for the increase in $(^{63}T_1T)^{-1}$ and that these fluctuations completely cancel for symmetry reason at the Hg site, so that Hg has only a Korringa behaviour. However this implies an antiferromagnetic coupling between different CuO_2 layers which is surprisingly strong (taking in particular into account the disorder induced by oxygen doping in the Hg planes). A puzzling ingredient to this question is provided by the NMR on $HgBa_2CaCu_2O_{6+\delta}$ [53]where the temperature dependence of $(T_1T)^{-1}$ for ^{63}Cu and ^{199}Hg is nearly the same. Clearly further experiments are needed to elucidate this point. Finally one has $^{199}T_1 \approx 10^2$. $^{63}T_1$, but it is much more difficult to obtain firm conclusions from a comparison of the magnitude of $^{63}T_1$ and $^{199}T_1$ since we deal with different nuclei, in contrast to YBCO.

We turn then to the Tl compounds. Again in $Tl_2Ba_2CuO_{6+\delta}$ [54,55]the Knight shift as well as the relaxation rate of ^{205}Tl display below T_c a strong drop, which shows that the wavefunction of superconducting electrons extends in a quite sizeable way to Tl nuclei. One may wonder, as for the Hg compounds, if this is not due to a transferred hyperfine interaction of the Hg nuclei with electrons on the Cu site of the nearby CuO_2 planes through the apical oxygen. This possibility remains to be investigated in details. However, just as in the Mila and Rice phenomenological analysis [56] for YBCO, one expects this hyperfine coupling to occur through the contact interaction due to Tl-s orbitals and therefore to be isotropic. The other contributions should be much smaller. However the spin part of the Knight shift has a sizeable anisotropy ($\approx 30\%$ in a $T_c = 110$K sample [55]), which is in contradiction with this hypothesis. Moreover, although it is difficult to obtain firm conclusions from magnitude considerations, it is rather striking to see that the ^{63}Cu and ^{205}Tl relaxation rates are nearly the same ($^{63}(1/T_1T) \approx 20\ sec^{-1}K^{-1}$ and $^{205}(1/T_1T) \approx 8\ sec^{-1}K^{-1}$ in the normal state [54,55]). Such a short $^{205}T_1$ is difficult to reconcile with a transferred hyperfine field. The natural interpretation of these ^{205}Tl NMR results is rather a confirmation of the two band picture given by band structure calculations.

Although more work is needed in order to reach a definite conclusion, we believe that the present NMR experimental evidence is leaning toward a two-band picture. However, even if we consider the single band hypothesis (assuming that only the CuO_2 band is relevant), the NMR shows unambiguously that the electronic wavefunction extends in a significant way to the Hg or Tl sites. Just as in our two band model, this provides a possible physical origin for an important Coulomb repulsion within this single band. This repulsion is likely to be quite anisotropic, since the probability of finding an electron on the Hg or Tl site will clearly change when one moves over the Fermi surface. This anisotropic repulsion might be responsible for a change of sign of the order parameter within this single band. Therefore in any case the NMR provides a clear hint that the Hg or Tl sites can not be safely omitted in a proper description of the electronic properties of the Hg or Tl compounds.

VI. NCCO AND LSCO

Let us finally consider the high Tc compounds, such as $La_{2-x}Sr_xCuO_4$ or $Nd_{2-x}Ce_xCuO_4$, which display only CuO_2 planes without any other possible metallic component and hence provide a check for our physical picture. Indeed in this case we are naturally led to a single band and naturally band structure calculations lead in these compounds to a single CuO_2 derived band [57]. In the framework of our model we do not expect any nodes in the gap. This leads for these compounds to s-wave pairing, even if it is quite possible that the order parameter is fairly anisotropic. The experimental evidence in $Nd_{2-x}Ce_xCuO_4$ is presently clearly in favor of s-wave pairing. Indeed the low temperature dependence of the penetration depth follows the standard weak coupling behaviour [58]. Tunneling [59] gives also a fairly standard BCS shape, and moreover the Eliashberg function extracted from these tunneling data leads to a T_c in good agreement with experiment, providing evidence for phonon mediated attractive interaction. Finally recent Raman scattering experiments [60] go also in the direction of s-wave pairing since the results can be explained by an almost isotropic gap. Therefore NCCO seems in contradiction with the spin fluctuation mechanism. The fact that it is an "electron doped" compound, in contrast with all the other "hole doped" compounds is a rather unconvincing explanation for this discrepancy. Indeed one starts with a Fermi liquid with strong spin fluctuations and it is not clear at all why a small change in doping, allowing to go from the hole doped side to the electron doped side, would kill these spin fluctuations or reduce strongly their coupling to the electrons, while at the same time a sizeable coupling to phonons would appear.

On the other hand the experimental situation is unclear in $La_{2-x}Sr_xCuO_4$ with some experiments in favor of s-wave and others in favor of nodes. To our knowledge there is no phase sensitive experiments, nor precise measurements of the low temperature behaviour of the penetration depth. Recent Raman scattering experiments [61] have found

results consistent with d-wave symmetry. However these results are not precise enough to prove convincingly the existence of nodes in the gap and some of their features do not agree with d-wave, but they display a clear anisotropy in the gap. Anyway, whatever the model, an experimental conclusion giving nodes in LSCO and no nodes in NCCO would be quite puzzling and we would rather hope for our understanding of high T_c superconductivity that both LSCO and NCCO fall in the same class, whatever it may be.

VII. CONCLUSION

In this paper we have proposed an extension to other high T_c compounds of a model introduced earlier for YBCO. This extension relies on the fact that a number of these compounds are believed to be "self-doped", with a part of the compound giving holes to CuO_2 planes. Explicitely this doping part corresponds to the BiO, HgO, TlO planes in BSCCO, HBCCO, TBCCO respectively, just as it is the CuO chains in YBCO. This doping part is then considered as inert or unimportant in many models. We propose instead that it is metallic, which leads naturally to a multiband model. This picture is supported by band structure calculations. Naturally these calculations can not make sure that these doping bands are indeed metallic, but they make this possibility quite plausible. The final answer on this point can only be obtained from experiment. We can then take over the ingredients of our model in YBCO, and assume a repulsive pairing interaction between these doping bands and the CuO_2 bands. This leads to an opposite sign for the order parameter on these bands and to nodes whenever the Fermi surfaces of these bands cross. We have considered in particular the case of BSCCO and shown that this model accounts with reasonable parameters for the low temperature dependence of the penetration depth. An interesting feature of BSCCO is that the nodes are not located near the 45^o direction found in the d-wave model. This is in contrast with YBCO where the location is not far from 45^o. Therefore the reliable experimental determination of the node locations is an important test for our model (we have discussed why ARPES does not provide a final answer in our view). We have then discussed the cases of HBCCO and TBCCO which have not been explored as much as BSCCO up to now. The situation in these compounds is somewhat similar to BSCCO with respect to our model. We have also considered the experimental evidence given by NMR and found that there are good indications for a metallic character of the doping bands in these last two compounds, although more experimental work is needed in order to get a definite anwer. Finally our model does not give nodes for NCCO and LSCO. This is in agreement with the present experimental situation for the first compound, but the evidence is quite ambiguous for the last one. We hope that experimental progress will allow fairly soon to confirm or invalidate our description. However whatever the answer we definitely need a consistent picture of all high T_c superconductors, in agreement with all experimental data.

VIII. ACKNOWLEDGEMENTS

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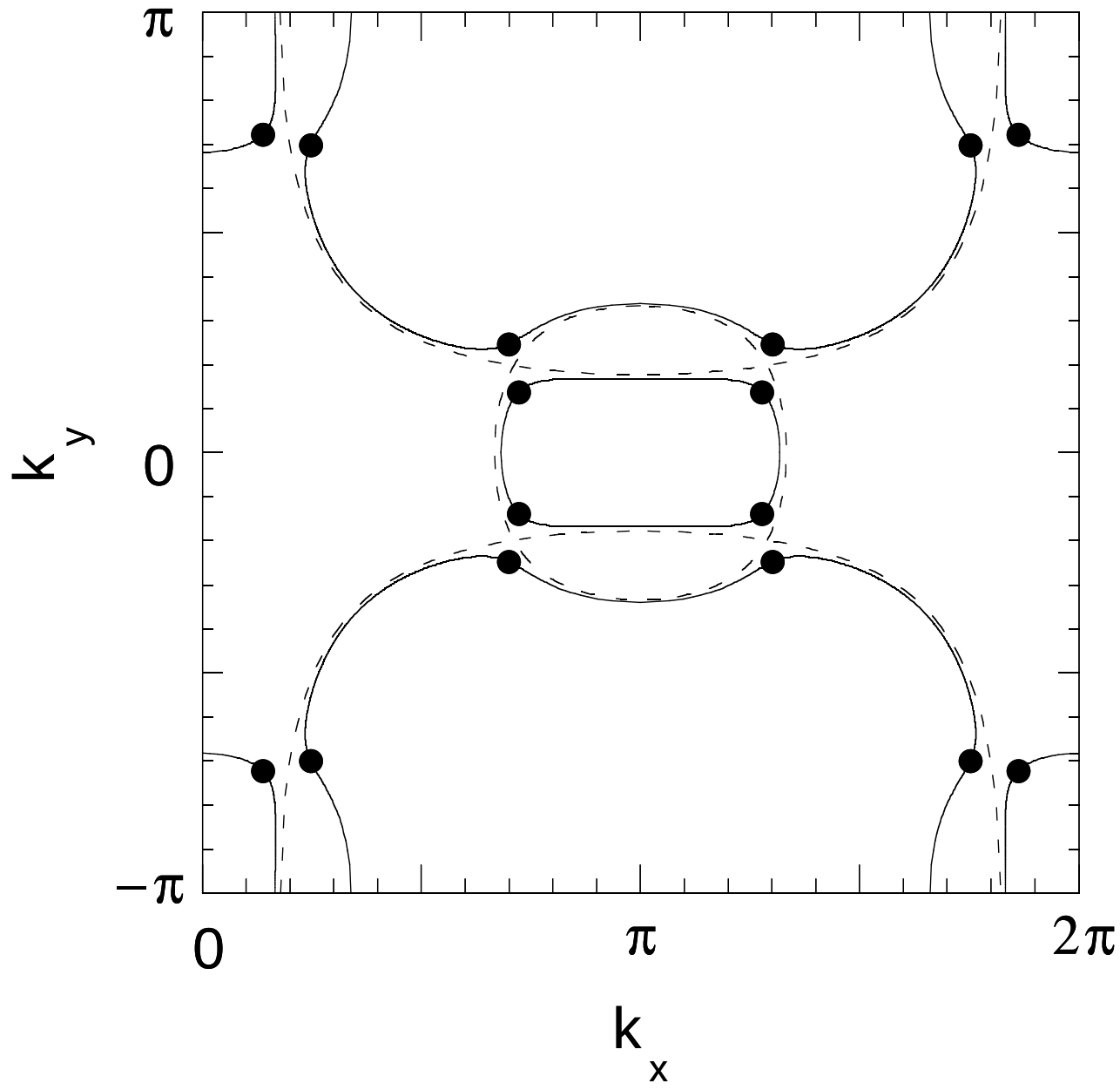
FIG. 1. Fermi surface in the Brillouin zone. The filled circles give the positions of the nodes of the gap.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